SCREENING-LEVEL HAZARD CHARACTERIZATION

SPONSORED CHEMICAL

Phosphorus Acid, Triphenyl Ester, Reaction Products with Dipropylene Glycol (CASRN 116265-68-0)

The High Production Volume (HPV) Challenge Program[1] was conceived as a voluntary initiative aimed at developing and making publicly available screening-level health and environmental effects information on chemicals manufactured in or imported into the United States in quantities greater than one million pounds per year. In the Challenge Program, producers and importers of HPV chemicals voluntarily sponsored chemicals; sponsorship entailed the identification and initial assessment of the adequacy of existing toxicity data/information, conducting new testing if adequate data did not exist, and making both new and existing data and information available to the public. Each complete data submission contains data on 18 internationally agreed to "SIDS" (Screening Information Data Set1[1,2]) endpoints that are screening-level indicators of potential hazards (toxicity) for humans or the environment.

The Environmental Protection Agency's Office of Pollution Prevention and Toxics (OPPT) is evaluating the data submitted in the HPV Challenge Program on approximately 1400 sponsored chemicals by developing hazard characterizations (HCs). These HCs consist of an evaluation of the quality and completeness of the data set provided in the Challenge Program submissions. They are not intended to be definitive statements regarding the possibility of unreasonable risk of injury to health or the environment.

The evaluation is performed according to established EPA guidance[2,3] and is based primarily on hazard data provided by sponsors; however, in preparing the hazard characterization, EPA considered its own comments and public comments on the original submission as well as the sponsor's responses to comments and revisions made to the submission. In order to determine whether any new hazard information was developed since the time of the HPV submission, a search of the following databases was made from one year prior to the date of the HPV Challenge submission to the present: (ChemID to locate available data sources including Medline/PubMed, Toxline, HSDB, IRIS, NTP, ATSDR, IARC, EXTOXNET, EPA SRS, etc.), STN/CAS online databases (Registry file for locators, ChemAbs for toxicology data, RTECS, Merck, etc.), Science Direct and ECHA[4]. OPPT's focus on these specific sources is based on their being of high quality, highly relevant to hazard characterization, and publicly available.

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[1] U.S. EPA. High Production Volume (HPV) Challenge Program; http://www.epa.gov/chemrtk/index.htm.
[2] U.S. EPA. HPV Challenge Program – Information Sources; http://www.epa.gov/chemrtk/pubs/general/guidocs.htm.
[3] U.S. EPA. Risk Assessment Guidelines; http://cfpub.epa.gov/ncea/raf/rafguid.cfm.
[4] European Chemicals Agency, http://echa.europa.eu.

OPPT does not develop HCs for those HPV chemicals which have already been assessed internationally through the HPV program of the Organization for Economic Cooperation and Development (OECD) and for which Screening Initial Data Set (SIDS) Initial Assessment Reports (SIAR) and SIDS Initial Assessment Profiles (SIAP) are available. These documents are presented in an international forum that involves review and endorsement by governmental authorities around the world. OPPT is an active participant in these meetings and accepts these documents as reliable screening-level hazard assessments.

These hazard characterizations are technical documents intended to inform subsequent decisions and actions by OPPT. Accordingly, the documents are not written with the goal of informing the general public. However, they do provide a vehicle for public access to a concise assessment of the raw technical data on HPV chemicals and provide information previously not readily available to the public.

Chemical Abstract Service Registry Number (CASRN)	**116265-68-0**
Chemical Abstract Index Name	**Phosphorus acid, triphenyl ester, reaction products with dipropylene glycol**
Structural Formula	**See Appendix**

Summary

Phosphorous acid, triphenyl ester, reaction products with dipropylene glycol is a liquid mixture of aryl phosphites that have negligible vapor pressure and negligible water solubility. The components of this mixture are expected to have low mobility in soil. Volatilization is expected to be low for the components of this mixture. The rate of hydrolysis is not known; however, phenyl phosphites have the potential to hydrolyze although hydrolysis may be a slow process due to a lack of water solubility. The rate of atmospheric photooxidation is rapid; however, this is not a relevant environmental degradation pathway since this substance is not expected to exist in the vapor phase in the atmosphere. Based upon very limited data, phosphorous acid, triphenyl ester, reaction products with dipropylene glycol is expected to have moderate persistence (P2) and high bioaccumulation potential (B3).

No adequate data are available on acute oral, repeated-dose, reproductive, developmental and genetic toxicity (gene mutations and chromosomal aberrations) endpoints with phosphorus acid, triphenyl ester, reaction products with dipropylene glycol.

No adequate data are available for the fish, aquatic invertebrates, and aquatic plants endpoints.

Acute oral, repeated-dose, reproductive, developmental and genetic toxicity (gene mutations and chromosomal aberrations) and the acute toxicity to fish and aquatic invertebrates and toxicity to aquatic plants endpoints were identified as data gaps under the HPV Challenge Program.

The sponsor, Chemtura Corporation, submitted a Test Plan and Robust Summaries to EPA for phosphorus acid, triphenyl ester, reaction products with dipropylene glycol (CASRN 116265-68-0; CA Index name: phosphorous acid, triphenyl ester, reaction products with dipropylene glycol) on December 25th, 2005. EPA posted the submission on the ChemRTK HPV Challenge website on January 25th, 2006 (http://www.epa.gov/oppt/chemrtk/pubs/summaries/phostries/c16116tc.htm). EPA comments on the original submission were posted to the website on April 14th, 2006, and comments on the revised submission were posted to the website on July 17th, 2008. Public comments were also received and posted to the website. The sponsor submitted updated/revised documents on November 10th, 2006, which were posted to the ChemRTK website on March 1st, 2007.

Substance Characterization

In the original submission the sponsor did not provide sufficient information on chemical characterization for the sponsored chemical − Phosphorus acid, triphenyl ester, reaction products with dipropylene glycol. The test plan did not indicate the test substance purity or information on the commercial product(s). EPA requested that the sponsor provide more complete compositional data for the test substance, including a range of molecular weights.

In its revised test plan, the sponsor provided additional information in IUCLID Data Set section 1.1.0; however, there is no clear statement of the range of structural composition of the sponsored substance, its average molecular weight, number of repeating units, possible isomeric complications, an approximate structural formula or variability of process formulations. The name "poly(dipropylene glycol) phenyl phosphite" alone provides insufficient structural information. The test plan states that the substance name "is intended to cover all the potential products derived from the reaction". The test plan needs to indicate what these potential products are in order to support an eventual hazard or risk characterization. Because the reaction yields a complex product, the test plan should discuss the reaction, its possible and known products including their structures and what subsequent treatment leads to the cited commercial products, Weston DHOP, Weston THOP and Weston PTP. In particular, in the IUCLID section 1.1.0, Weston THOP is characterized as 30 – 60% tetraphenyl dipropyleneglycol "diphosphate" (probably intended to be the diphosphite), a monomer that would be at the low end of the spectrum of possible products and therefore, an important component of the sponsored substance. However, it is impossible to determine from the submission whether this substance is a significant component of the sponsored substance. In addition, the CAS number assigned by the sponsor is for an oligomeric substance, not for a monomer.

Although the sponsor planned significant testing, EPA indicated that it would be difficult to evaluate the utility and the results of the proposed testing because it is unclear whether potential impurities such as trimeric or higher molecular-weight polyglycol substances, bridged diphosphites, or partially reacted aryl alkyl phosphites are present in significant amounts. For aquatic toxicity endpoints, the quantity of any higher molecular-weight components would help determine the need for chronic vs. acute toxicity testing.

Supporting Chemicals

The sponsor indicated that the two proposed supporting chemicals are contained in commercial products Weston DHOP and THOP (which includes CASRN 80584-86-7, poly(dipropyleneglycol)triphosphite) and PTP (which includes CASRN 13474-96-9, heptakis(dipropyleneglycol)triphosphite) that themselves are derived from the sponsored substance and states that “Data from these potential products are relevant for the sponsored substance...” The mere assertion of relevance is inadequate for the purposes of the HPV Challenge Program. There is no structural comparison or other information presented to support a relationship to the sponsored chemical. In addition, the data provided show vastly different physicochemical properties (Table 2 in the revised test plan) for these two substances and it is not clear which one (if either) would better represent the sponsored chemical.

There is much confusion in the submission as to the identity of the supporting chemical having CASRN 80584-86-7. The substance is incorrectly named in the test plan and throughout the robust summaries as a phosphate rather than a phosphite. Only in the IUCLID section 1.1.0 the substance is properly named, but in the same paragraph, the CASRNs associated with two other names, are both incorrect.

1. Chemical Identity

1.1 Identification and Purity

Phosphorous acid, triphenyl ester, reaction products with dipropylene glycol is a liquid with negligible vapor pressure and negligible water solubility.

1.2 Physical-Chemical Properties

The physical-chemical properties of phosphorous acid, triphenyl ester, reaction products with dipropylene glycol are summarized in Table 1. The structure of the compound is provided in the Appendix.

Table 1. Physical-Chemical Properties of Phosphorous acid, triphenyl ester, reaction products with dipropylene glycol and Supporting Chemicals[1,2]

Property	Phosphorous acid, triphenyl ester, reaction products with dipropylene glycol	Heptakis(dipropyleneglycol) triphosphite (supporting chemical)	Poly(dipropylene glycol) phenyl phosphite (supporting chemical)
CASRN	116265-68-0	13474-96-9	80584-86-7
Molecular Weight	566 (typical)	1023 (typical)	823 (typical)
Physical State	Liquid	Liquid	Yellow liquid
Melting Point	No data[3]	No data[3]	No data[3]
Boiling Point	>300°C (estimated)[4]	>300°C (estimated)[4]	>300°C (estimated)[4]
Vapor Pressure	$<1.0\times10^{-10}$ mm Hg at 25°C (estimated)[4]	$<1.0\times10^{-10}$ mm Hg at 25°C (estimated)[4]	$<1.0\times10^{-10}$ mm Hg at 25°C (estimated)[4]
Dissociation Constant	Not applicable	Not applicable	Not applicable
Henry's Law Constant	$<1.0\times10^{-10}$ atm-m^3/mole at 25°C (estimated)[4]	$<1.0\times10^{-10}$ atm-m^3/mole at 25°C (estimated)[4]	$<1.0\times10^{-10}$ atm-m^3/mole at 25°C (estimated)[4]
Water Solubility	1.3×10^{-5} mg/L at 25°C (estimated)[4]	185 mg/L at 25°C (estimated)[4]	5.6×10^{-9} mg/L at 25°C (estimated)[4]
Log K_{ow}	8.57 (estimated)[4]	-3.41 (estimated)[4]	10.51 (estimated)[4]

[1]Chemtura Corporation. 2006. Revised Test Plan and Robust Summary for Phosphorous acid, triphenyl ester, reaction products with dipropylene glycol. Available online at http://www.epa.gov/oppt/chemrtk/pubs/summaries/phostries/c16116tc.htm as of June 25, 2012.

[2]Estimates based on SMILES notations for representative structures given in the Appendix. CASRN 116265-68-0: c1(OP(Oc2ccccc2)OC(C)COCC(C)OP(Oc2ccccc2)Oc2ccccc2)ccccc1; CASRN 13474-96-9: C(C)(COC(C)CO)OP(OC(C)COCC(C)OP(OC(C)COCC(C)OP(OC(C)COCC(C)O)OC(C)COCC(C)O)OC(C)COCC(C)O)OC(C)COCC(C)O; CASRN 80584-86-7; c1(OP(Oc2ccccc2)OC(C)COC(C)COP(Oc2ccccc2)OC(C)COCC(C)OP(Oc2ccccc2)Oc2ccccc2)ccccc1.

[3]The mixture will not have a well-defined melting point; since the substance is a liquid, it can be assumed to melt at <25°C.

[4] U.S. EPA. 2012. Estimation Programs Interface Suite™ for Microsoft® Windows, v4.10. U.S. Environmental Protection Agency, Washington, DC, USA. Available online at http://www.epa.gov/opptintr/exposure/pubs/episuitedl.htm as of June 25, 2012.

2. General Information on Exposure

2.1 Production Volume and Use

CASRN 116265-68-0 had an aggregated production and/or import volume in the United States between 500,000 pounds to 1 million pounds during calendar year 2005.

Non-confidential information in the IUR indicated that the industrial processing and uses of the chemical include resin and synthetic rubber manufacturing as stabilizers. No commercial and consumer uses were reported for the chemical.

2.2 Environmental Exposure and Fate

The components of phosphorous acid, triphenyl ester, reaction products with dipropylene glycol are expected to possess low mobility in soil. No biodegradation studies were available for this compound or the supporting substances. Volatilization is expected to be low for the components of phosphorous acid, triphenyl ester, reaction products with dipropylene glycol. The rate of hydrolysis is not known but phenyl phosphites have the potential to hydrolyze. However, the low water solubility of this substance may attenuate this process. The rate of atmospheric photooxidation is rapid; however, this is not a relevant environmental degradation pathway since this substance is not expected to exist in the vapor phase in the atmosphere. An estimated bioaccumulation factor (BAF) for a lower molecular weight representative aryl phosphite suggests that components of this mixture may bioaccumulate. Phosphorous acid, triphenyl ester, reaction products with dipropylene glycol is expected to have moderate persistence (P2) and high bioaccumulation potential (B3).

The environmental fate characteristics of phosphorous acid, triphenyl ester, reaction products with dipropylene glycol are summarized in Table 2.

Table 2. Environmental Properties of of Phosphorous acid, triphenyl ester, reaction products with dipropylene glycol and Supporting Chemicals[1,2]

Property	Phosphorous acid, triphenyl ester, reaction products with dipropylene glycol	Heptakis(dipropylene glycol) triphosphite (supporting chemical)	Poly(dipropylene glycol) phenyl phosphite (supporting chemical)
CASRN	116265-68-0	13474-96-9	80584-86-7
Photodegradation Half-life	1.0 hours (estimated)[3]	13.1 hours (estimated)[3]	0.6 hours (estimated)[3]
Hydrolysis Half-life	No data	Slowly hydrolyzes	No data
Biodegradation	No data	No data	No data
Bioaccumulation Factor	BAF = 6,337 (estimated)[3]	BAF = 0.89 (estimated)[3]	BAF = 695 (estimated)[3]
Log K_{oc}	9.7 (estimated)[3]	8.0 (estimated)[3]	13.1 (estimated)[3]
Fugacity (Level III Model)[3]			
Air (%)	<0.1	<0.1	<0.1
Water (%)	1.3	0.6	0.7
Soil (%)	31.6	52.1	40.8
Sediment (%)	67.1	47.3	58.4
Persistence[4]	P2 (moderate)	P2 (moderate)	P2 (moderate)
Bioaccumulation[4]	B3 (high)	B1 (low)	B1 (low)

[1]Chemtura Corporation. 2006. Revised Test Plan and Robust Summary for Phosphorous acid, triphenyl ester, reaction products with dipropylene glycol. Available at http://www.epa.gov/oppt/chemrtk/pubs/summaries/phostries/c16116tc.htm as of June 25, 2012.

[2]Estimates based on SMILES notations for representative structures given in the Appendix. CASRN 116265-68-0: c1(OP(Oc2ccccc2)OC(C)COCC(C)OP(Oc2ccccc2)Oc2ccccc2)ccccc1; CASRN 13474-96-9: C(C)(COC(C)CO)OP(OC(C)COCC(C)OP(OC(C)COCC(C)OP(OC(C)COCC(C)O)OC(C)COCC(C)O)OC(C)COCC(C)O)OC(C)COCC(C)O; CASRN 80584-86-7; c1(OP(Oc2ccccc2)OC(C)COC(C)COP(Oc2ccccc2)OC(C)COCC(C)OP(Oc2ccccc2)Oc2ccccc2)ccccc1

[3]U.S. EPA. 2012. Estimation Programs Interface Suite™ for Microsoft® Windows, v4.10. U.S. Environmental Protection Agency, Washington, DC, USA. Available online at http://www.epa.gov/opptintr/exposure/pubs/episuitedl.htm as of June 25, 2012.

[4]Federal Register. 1999. Category for Persistent, Bioaccumulative, and Toxic New Chemical Substances. *Federal Register* 64, Number 213 (November 4, 1999) pp. 60194–60204.

Conclusion: Phosphorous acid, triphenyl ester, reaction products with dipropylene glycol is a liquid mixture of aryl phosphites that have negligible vapor pressure and negligible water solubility. The components of this mixture are expected to have low mobility in soil. Volatilization is expected to be low for the components of this mixture. The rate of hydrolysis is not known; however, phenyl phosphites have the potential to hydrolyze although hydrolysis may be a slow process due to a lack of water solubility. The rate of atmospheric photooxidation is rapid; however, this is not a relevant environmental degradation pathway since this substance is not expected to exist in the vapor phase in the atmosphere. Based upon very limited data, phosphorous acid, triphenyl ester, reaction products with dipropylene glycol is expected to have moderate persistence (P2) and high bioaccumulation potential (B3).

3. Human Health Hazard

Acute Oral Toxicity

No adequate data.

Data for the proposed supporting chemicals were submitted for this endpoint. However, insufficient justification for the use of these data was provided. Further, an evaluation of the MSDS for these substances shows that the sponsored substance is not present in these commercial substances excepting for WESTON® PTP (Version 1.0, Revision Date 12/07/2010: http://www.chemtura.com/msd/external/e/result/result_main_fs.jsp?C003=EN&P_SSN=104104&C002=NA-US-SDS&C001=MSDS&P_LANGU=E&C999=X&submit=Continue&P_SYS=6&C013=&myopt=WESTON+PTP&C014=WESTON*PTP&submit=Submit). The MSDS for WESTON® PTP identifies the sponsored substance (CASRN 116265-68-0) as a component. However, another component [CASRN 13474-96-9; Heptakis (dipropyleneglycol)triphosphite] for this proposed supporting chemical is identified in the test plan but is not noted in the MSDS for WESTON® PTP, further adding to the confusion over the appropriateness of the use of data for the proposed supporting chemicals.

Repeated-Dose, Reproductive and Developmental Toxicity

No data.

Genetic Toxicity – Gene Mutation and Chromosomal Aberrations

No data.

Conclusion: No adequate data are available on acute oral, repeated-dose, reproductive, developmental and genetic toxicity (gene mutations and chromosomal Aberrations) with phosphorus acid, triphenyl ester, reaction products with dipropylene glycol.

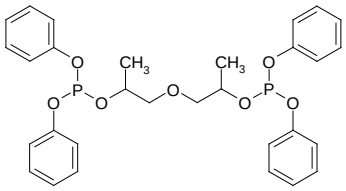
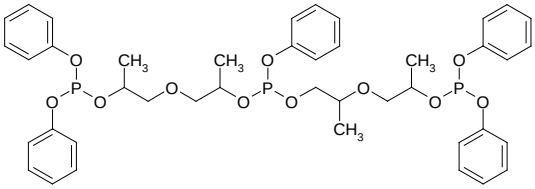
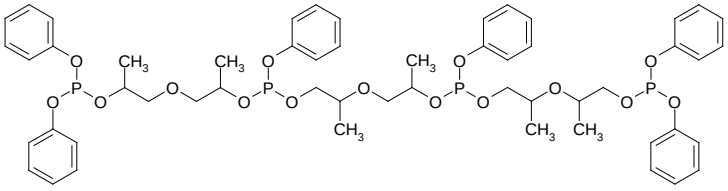
4. Hazard to the Environment

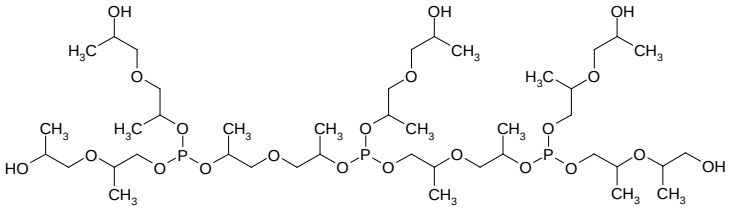
Acute Toxicity to Fish and Aquatic Invertebrates and Toxicity to Aquatic Plants

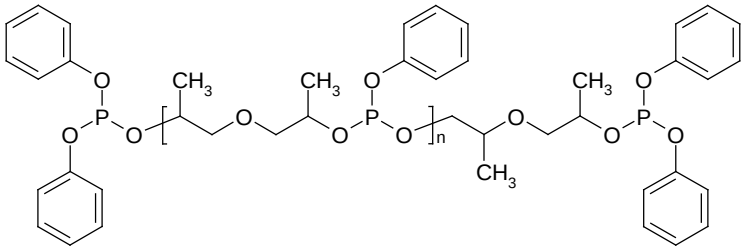
No adequate data are available for the fish, aquatic invertebrates, and aquatic plants endpoints.

Conclusion: No adequate data are available for the fish, aquatic invertebrates, and aquatic plants endpoints.

APPENDIX

Sponsored Chemical		
Chemical Name	**CASRN**	**Representative Structure[1]**
Phosphorous acid, triphenyl ester, reaction products with dipropylene glycol	116265-68-0	Representative structures for the sponsored chemical 'Phosphorous acid, triphenyl ester, reaction products with dipropylene glycol'  Molecular Weight =566.53 Exact Mass =566 Molecular Formula =C30H32O7P2 Molecular Composition =C 63.60% H 5.69% O 19.77% P 10.93%  Molecular Weight =822.77 Exact Mass =822 Molecular Formula =C42H49O11P3 Molecular Composition =C 61.31% H 6.00% O 21.39% P 11.29%  Molecular Weight =1079.01 Exact Mass =1078 Molecular Formula =C54H66O15P4 Molecular Composition =C 60.11% H 6.17% O 22.24% P 11.48%

Supporting Chemicals		
Chemical Name	**CASRN**	**Representative Structure[1]**
Bis[13-Hydroxy-7-[2-(2-hydroxypropoxy)-1-methylethoxy]-1,5,9-trimethyl-3,6,8,11-tetraoxa-7-phosphatetradec-1-yl][2-(2-hydroxypropoxy)-1-methylethyl]phosphine	13474-96-9	 Representative structure of 'heptakis(dipropyleneglycol) triphosphite' The CAS number 13474-96-9 is a close match for this description.

Supporting Chemicals		
Chemical Name	**CASRN**	**Representative Structure[1]**
Oxybispropylenebis[(1,5,9,13,17,21-hexamethyl-7,15,23,23-tetraphenoxy-3,6,8,11,14,16,19,22-octaoxa-7,15,23-triphosphatricos-1-yl)(phenyl)phosphine]	80584-86-7	 Representative structure for 'poly(dipropylene glycol) phenyl phosphite' The CAS number '80584-86-7' does not match the description or structure'

[1]Sponsor did not verify the identity of these structures. There is no clear statement of the range of structural composition of the sponsored substance, its average molecular weight, or possible isomeric forms in the test plan or summaries. Representative structures were developed using the limited information provided in the test plan. The two supporting substances are not listed on the public TSCA inventory.